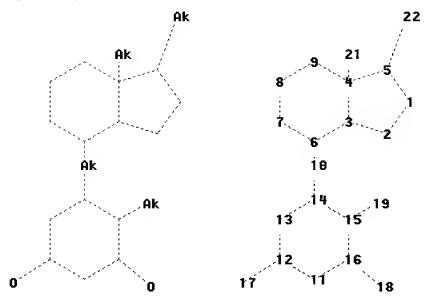
## Structures uploaded into STN REGISTRY

Uploading L3.str



```
chain nodes :
10  17  18  19  21  22
ring nodes :
1  2  3  4  5  6  7  8  9  11  12  13  14  15  16
chain bonds :
4-21  5-22  6-10  10-14  12-17  15-19  16-18
ring bonds :
1-2  1-5  2-3  3-4  3-6  4-5  4-9  6-7  7-8  8-9  11-12  11-16  12-13  13-14  14-15
15-16
exact/norm bonds :
1-2  1-5  2-3  3-4  3-6  4-5  4-9  4-21  5-22  6-7  6-10  7-8  8-9  10-14  11-12
11-16  12-13  12-17  13-14  14-15  15-16  15-19  16-18
isolated ring systems :
containing 1 : 11 :
```

## Connectivity:

17:1 E exact RC ring/chain 18:1 E exact RC ring/chain
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom

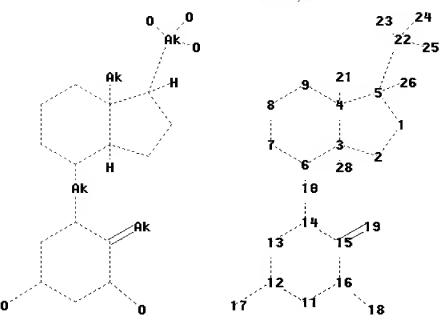
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS 21:CLASS

Generic attributes :

22:

Type of chain : Branched Saturation : Saturated

Uploading L9.str



```
chain nodes :
10 17 18 19 21 22 23 24 25
                                         26
ring nodes :
1 2 3 4 5 6 7 8
                            9
                                11
                                     12
                                          13
                                             14 15
chain bonds :
3-28 4-21 5-22 5-26 6-10
                                   10-14 12-17 15-19
                                                            16-18 22-23 22-24 22-25
ring bonds :
1-2 1-5 2-3 3-4 3-6
                            4-5
                                   4-9 6-7 7-8 8-9 11-12 11-16
                                                                            12-13 13-14 14-15
15-16
exact/norm bonds :
1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 3-6 \quad 3-28 \quad 4-5 \quad 4-9 \quad 4-21 \quad 5-22 \quad 5-26 \quad 6-7 \quad 6-10
                                                                                   7-8 8-9 10-
11 - 12 \quad 11 - 16 \quad 12 - 13 \quad 12 - 17 \quad 13 - 14 \quad 14 - 15 \quad 15 - 16 \quad 15 - 19 \quad 16 - 18 \quad 22 - 23 \quad 22 - 24 \quad 22 - 25
isolated ring systems :
containing 1 : 11 :
```

#### Connectivity :

17:1 E exact RC ring/chain 18:1 E exact RC ring/chain 19:1 E exact RC ring/chain 23:1 E exact RC ring/chain 24:1 E exact RC ring/chain 25:1 E exact RC ring/chain Match level:

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS

23:CLASS 24:CLASS 25:CLASS 26:CLASS 28:CLASS

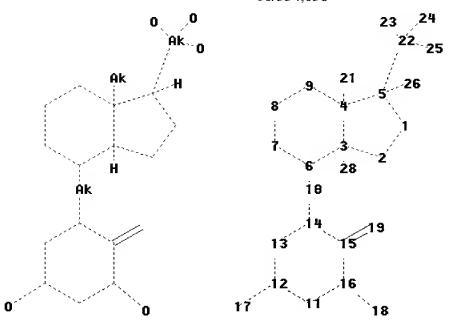
Generic attributes :

19:

Number of Carbon Atoms : less than 7

22:

Type of chain : Branched Saturation : Saturated Number of Carbon Atoms : 7 or more



chain nodes :

Node 22: Limited

```
10 17 18 19 21 22 23 24 25
                                 26
ring nodes :
1 2 3 4 5
             6 7 8
                      9 11 12
                                 13
                                    14 15
chain bonds :
3-28 4-21 5-22 5-26 6-10
                            10-14 12-17 15-19
                                                 16-18 22-23 22-24 22-25
ring bonds :
1-2 1-5 2-3 3-4 3-6 4-5
                             4-9 6-7 7-8 8-9 11-12 11-16
                                                              12-13 13-14 14-15
15-16
exact/norm bonds :
1-2 1-5 2-3 3-4 3-6 3-28 4-5 4-9 4-21 5-22 5-26 6-7 6-10
                                                                    7-8 8-9 10-
11-12 \quad 11-16 \quad 12-13 \quad 12-17 \quad 13-14 \quad 14-15 \quad 15-16 \quad 16-18 \quad 22-23 \quad 22-24 \quad 22-25
exact bonds :
15-19
isolated ring systems :
containing 1 : 11 :
Connectivity :
11:2 E exact RC ring/chain 17:1 E exact RC ring/chain 18:1 E exact RC ring/chain
19:1 E exact RC ring/chain 23:1 E exact RC ring/chain 24:1 E exact RC ring/chain
25:1 E exact
RC ring/chain
Match level:
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS
21:CLASS 22:CLASS
23:CLASS 24:CLASS 25:CLASS 26:CLASS 28:CLASS
Generic attributes :
22:
Type of chain
                      : Branched
Saturation
                      : Saturated
Number of Carbon Atoms: 7 or more
Element Count :
```

C, C9

Uploading L20.str 23 24 22. <sub>25</sub> Ak 21 -26 Н 28 10 Ak .12 17 chain nodes : 10 17 18 19 21 22 23 24 25 26 ring nodes : 1 2 3 4 5 6 7 8 9 11 12 13 14 15 16 chain bonds : 3-28 4-21 5-22 5-26 6-10 10-14 12-17 15-19 16-18 22-23 22-24 22-25ring bonds :  $1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 3-6 \quad 4-5 \quad 4-9 \quad 6-7 \quad 7-8 \quad 8-9 \quad 11-12 \quad 11-16 \quad 12-13 \quad 13-14 \quad 14-15$ 15-16 exact/norm bonds :  $1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 3-6 \quad 3-28 \quad 4-5 \quad 4-9 \quad 4-21 \quad 5-22 \quad 5-26 \quad 6-7 \quad 6-10$  $11-12 \quad 11-16 \quad 12-13 \quad 12-17 \quad 13-14 \quad 14-15 \quad 15-16 \quad 16-18 \quad 22-23 \quad 22-24$ exact bonds : 15 - 19isolated ring systems : containing 1 : 11 : Connectivity: 11:2 E exact RC ring/chain 17:1 E exact RC ring/chain 18:1 E exact RC ring/chain 19:1 E exact RC ring/chain 22:4 E exact RC ring/chain 23:1 E exact RC ring/chain 24:1 E exact RC ring/chain 25:1 E exact RC ring/chain Match level: 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 28:CLASS Generic attributes :

22:

Type of chain : Branched Saturation : Saturated Number of Carbon Atoms : 7 or more

Element Count : Node 22: Limited C,C9

Uploading L24.str



chain nodes : 10 17 18 20 21 22 24 26 28 29 30 31 32 33 ring nodes : 1 2 3 4 5 6 7 8 9 11 12 13 14 15 16 chain bonds :  $3-24 \quad 4-20 \quad 5-21 \quad 6-10 \quad 10-14 \quad 12-17 \quad 16-18 \quad 21-22 \quad 21-28 \quad 22-26 \quad 29-31 \quad 29-32 \quad 30-129 \quad 29-31 \quad 29-3$ 33 ring bonds :  $1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 3-6 \quad 4-5 \quad 4-9 \quad 6-7 \quad 7-8 \quad 8-9 \quad 11-12 \quad 11-16 \quad 12-13 \quad 13-14 \quad 14-15$ 15 - 16exact/norm bonds :  $1-2 \quad 1-5 \quad 2-3 \quad 3-4 \quad 3-6 \quad 3-24 \quad 4-5 \quad 4-9 \quad 4-20 \quad 5-21 \quad 6-7 \quad 6-10 \quad 7-8 \quad 8-9 \quad 10-14$ 11-12 11-16 12-13 12-17 13-14 14-15 15-16 16-18 21-22 21-28 22-26 29-31 29-32 30-33 isolated ring systems : containing 1 : 11 :

G1:[\*1],[\*2]

Connectivity:

11:2 E exact RC ring/chain 21:4 E exact RC ring/chain 33:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 20:CLASS 21:CLASS

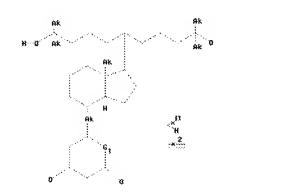
24:CLASS 26:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS Generic attributes :

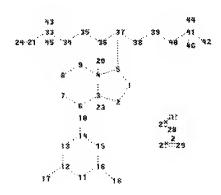
21:

Type of chain : Branched Number of Carbon Atoms : 7 or more

Element Count : Node 21: Limited C,C9

Uploading L31.str





chain nodes :

ring nodes :

1 2 3 4 5 6 7 8 9 11 12 13 14 15 16

chain bonds :

3-23 4-20 5-37 6-10 10-14 12-17 16-18 21-24 21-33 25-27 25-28 26-29 33-34

33-43 33-45 34-35 35-36 36-37 37-38 38-39 39-40 40-41 41-42 41-44 41-46 ring bonds:

exact/norm bonds :

 $33-45 \quad 34-35 \quad 35-36 \quad 36-37 \quad 37-38 \quad 38-39 \quad 39-40 \quad 40-41 \quad 41-42 \quad 41-44 \quad 41-46 \quad 41-4$ 

37:CLASS 38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS 43:CLASS 44:CLASS

45:CLASS 46:CLASS

# Full search history

=> d his full (FILE 'HOME' ENTERED AT 15:18:59 ON 31 JUL 2009) FILE 'REGISTRY' ENTERED AT 15:19:22 ON 31 JUL 2009 L1STRUCTURE UPLOADED D L1 L20 SEA SSS SAM L1 FILE 'STNGUIDE' ENTERED AT 15:20:05 ON 31 JUL 2009 FILE 'REGISTRY' ENTERED AT 15:21:11 ON 31 JUL 2009 L3 STRUCTURE UPLOADED D L3 3 SEA SSS SAM L3 L4D SCAN 1106 SEA SSS FUL L3 L5SAVE TEMP L5 GOO038STL3/A 1 SEA SUB=L5 SSS SAM L1 L6 D SCAN L7 57 SEA SUB=L5 SSS FUL L1 FILE 'HCAPLUS' ENTERED AT 15:24:18 ON 31 JUL 2009 81 SEA SPE=ON ABB=ON PLU=ON L7 L8 FILE 'STNGUIDE' ENTERED AT 15:24:29 ON 31 JUL 2009 FILE 'REGISTRY' ENTERED AT 15:27:32 ON 31 JUL 2009 L9 STRUCTURE UPLOADED D L9 1 SEA SUB=L5 SSS SAM L9 L10 D SCAN 46 SEA SUB=L5 SSS FUL L9 L12 7 SEA SPE=ON ABB=ON PLU=ON L11 AND F/ELS 39 SEA SPE=ON ABB=ON PLU=ON L11 NOT L12 L13 FILE 'HCAPLUS' ENTERED AT 15:31:02 ON 31 JUL 2009 74 SEA SPE=ON ABB=ON PLU=ON L13 L14 FILE 'STNGUIDE' ENTERED AT 15:31:16 ON 31 JUL 2009 FILE 'REGISTRY' ENTERED AT 15:35:08 ON 31 JUL 2009 L15 STRUCTURE UPLOADED D L15 1 SEA SUB=L5 SSS SAM L15 L16 D SCAN L17 19 SEA SUB=L5 SSS FUL L15 D SCAN FILE 'HCAPLUS' ENTERED AT 15:37:31 ON 31 JUL 2009 18 SEA SPE=ON ABB=ON PLU=ON L17 L18 FILE 'REGISTRY' ENTERED AT 15:37:45 ON 31 JUL 2009 L19 19 SEA SPE=ON ABB=ON PLU=ON L13 AND L17 L20 STRUCTURE UPLOADED D L20

1 SEA SUB=L19 SSS SAM L20

L21

D SCAN L22 8 SEA SUB=L19 SSS FUL L20 D SCAN FILE 'HCAPLUS' ENTERED AT 15:41:26 ON 31 JUL 2009 L23 13 SEA SPE=ON ABB=ON PLU=ON L22 D L23 1-13 TI D L23 1-13 AU FILE 'STNGUIDE' ENTERED AT 15:43:05 ON 31 JUL 2009 FILE 'REGISTRY' ENTERED AT 15:49:37 ON 31 JUL 2009 L24 STRUCTURE UPLOADED L25 1 SEA SSS SAM L24 D SCAN L26 194 SEA SSS FUL L24 L27 176 SEA SPE=ON ABB=ON PLU=ON L26 NOT L5 176 SEA SPE=ON ABB=ON PLU=ON L27 NOT L22 L28 176 SEA SPE=ON ABB=ON PLU=ON L28 NOT L17 L29 FILE 'HCAPLUS' ENTERED AT 15:52:37 ON 31 JUL 2009 41 SEA SPE=ON ABB=ON PLU=ON L29 L30 D L30 41 FHITSTR FILE 'STNGUIDE' ENTERED AT 15:53:49 ON 31 JUL 2009 FILE 'REGISTRY' ENTERED AT 15:58:43 ON 31 JUL 2009 STRUCTURE UPLOADED L31 D L31 L32 1 SEA SUB=L26 SSS SAM L31 D SCAN L33 10 SEA SUB=L26 SSS FUL L31 L34 5 SEA SPE=ON ABB=ON PLU=ON L33 NOT L5 D SCAN D SCAN L33 L35 5 SEA SPE=ON ABB=ON PLU=ON L33 AND L5 L36 10 SEA SPE=ON ABB=ON PLU=ON L34 OR L35 10 SEA SPE=ON ABB=ON PLU=ON L36 AND L33 L37 4 SEA SPE=ON ABB=ON PLU=ON L23 AND L37 L38 FILE 'HCAPLUS' ENTERED AT 16:03:42 ON 31 JUL 2009 11 SEA SPE=ON ABB=ON PLU=ON L37 L39 L40 11 SEA SPE=ON ABB=ON PLU=ON L34 L41 11 SEA SPE=ON ABB=ON PLU=ON L35 11 SEA SPE=ON ABB=ON PLU=ON L38 L42 11 SEA SPE=ON ABB=ON PLU=ON (L39 OR L40 OR L41 OR L42) L43 11 SEA SPE=ON ABB=ON PLU=ON L23 AND L43 L44L4513 SEA SPE=ON ABB=ON PLU=ON L23 OR L43 L46 18 SEA SPE=ON ABB=ON PLU=ON L19 L47 5 SEA SPE=ON ABB=ON PLU=ON L46 NOT L45 D L47 1-5 TI FILE 'HCAPLUS' ENTERED AT 16:09:52 ON 31 JUL 2009 D L47 1-5 TI D L47 1-5 AU L48 13 SEA SPE=ON ABB=ON PLU=ON (L43 OR L44 OR L45) SAVE TEMP L48 GOO038STL48/A E ADORINI L?/AU 272 SEA SPE=ON ABB=ON PLU=ON ADORINI L?/AU L49

E PENNA G?/AU

```
L50
            74 SEA SPE=ON ABB=ON PLU=ON PENNA G?/AU
               E MAEHR H?/AU
L51
            96 SEA SPE=ON ABB=ON PLU=ON MAEHR H?/AU
             5 SEA SPE=ON ABB=ON PLU=ON L49 AND L50 AND L51
L52
            70 SEA SPE=ON ABB=ON PLU=ON L49 AND (L50 OR L51) 5 SEA SPE=ON ABB=ON PLU=ON L50 AND L51
L53
L54
L55
            63 SEA SPE=ON ABB=ON PLU=ON (L49 OR L50 OR L51) AND BIOXELL?/CO
               ,CS,PA,SO
            76 SEA SPE=ON ABB=ON PLU=ON (L49 OR L50 OR L51) AND (VITAMIN(W)
L56
               D OR "VITAMIN D" OR (VITAMIN? (4A) (DERIV? OR ANALOG? OR MIMIC?
               OR MODIF?)) OR (VITAMIN(W)(D3 OR D4)))
            40 SEA SPE=ON ABB=ON PLU=ON L55 AND L56
L57
            45 SEA SPE=ON ABB=ON PLU=ON (L52 OR L53 OR L54) AND (L55 OR
L58
               L56)
L59
            25 SEA SPE=ON ABB=ON PLU=ON L57 AND L58
L60
            26 SEA SPE=ON ABB=ON PLU=ON L52 OR L59
               D L60 1-11 TI
            10 SEA SPE=ON ABB=ON PLU=ON (L57 OR L58) AND (CALCIFER? OR
L61
               CHOLECALCIFER? OR CHOLE(W)CALCIFER?)
            33 SEA SPE=ON ABB=ON PLU=ON (L60 OR L61)
L62
    FILE 'MEDLINE, BIOSIS, EMBASE, DRUGU' ENTERED AT 16:17:50 ON 31 JUL 2009
             7 SEA SPE=ON ABB=ON PLU=ON L54
             7 SEA SPE=ON ABB=ON PLU=ON L52
L64
           181 SEA SPE=ON ABB=ON PLU=ON L53
L65
            96 SEA SPE=ON ABB=ON PLU=ON L57
L66
           112 SEA SPE=ON ABB=ON PLU=ON L58
L67
            22 SEA SPE=ON ABB=ON PLU=ON (L65 OR L66 OR L67) AND (CALCIFER?
L68
               OR CHOLECALCIFER? OR CHOLE(W) CALCIFER?)
L69
            55 SEA SPE=ON ABB=ON PLU=ON L66 AND L67
            55 SEA SPE=ON ABB=ON PLU=ON (L63 OR L64 OR L65) AND L69
L70
            29 SEA SPE=ON ABB=ON PLU=ON L64 OR L68
L71
            55 SEA SPE=ON ABB=ON PLU=ON L70 AND (VITAMIN(W) D OR "VITAMIN
L72
               D" OR (VITAMIN?(4N)(DERIV? OR ANALOG? OR MIMIC? OR MODIF?)) OR
               (VITAMIN(W)(D3 OR D4)))
            56 SEA SPE=ON ABB=ON PLU=ON L60
L73
L74
            55 SEA SPE=ON ABB=ON PLU=ON L72 AND L73
            14 SEA SPE=ON ABB=ON PLU=ON L71 AND (L73 OR L74)
L75
            29 SEA SPE=ON ABB=ON PLU=ON L71 OR L75
L76
    FILE 'STNGUIDE' ENTERED AT 16:23:43 ON 31 JUL 2009
    FILE 'HCAPLUS' ENTERED AT 16:24:43 ON 31 JUL 2009
               D STAT OUERY L48
               D L48 1-13 IBIB ED ABS HITRN HITSTR
               D QUE L62
               D QUE L76
    FILE 'HCAPLUS, MEDLINE, BIOSIS, EMBASE, DRUGU' ENTERED AT 16:27:00 ON 31
    JUL 2009
L77
            40 DUP REM L62 L76 (22 DUPLICATES REMOVED)
                    ANSWERS '1-33' FROM FILE HCAPLUS
                    ANSWERS '34-35' FROM FILE MEDLINE
                    ANSWERS '36-37' FROM FILE EMBASE
                    ANSWERS '38-40' FROM FILE DRUGU
```

FILE HOME

D L77 1-40 IBIB ABS